6. COMPUTER MODELLING OF THE QUASI-CRYSTALLOID BIOPOLYMER STRUCTURE II.

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Abstract

During our previous investigations (1995) on the structure and symmetry of the biopolymer system of the partially degraded plant cell wall we have recognized that a part of the problems can be resolved exclusively by computer modelling. Another research program was projected in our laboratory, based on two opposite statepoints as follows. 1. The computer modelling of the biopolymer structures based on TEM observations. 2. Presumed or hypothetical structures which, till this time have not been observed on biological objects. This contribution presents the first computer modelling of a "nonsense" spherical calotte composed of regular pentagon units.

Key words: Plant cell wall, biopolymer system, computer modelling.

Introduction

A long time ago it was established that the sphere is the most perfect figure, because every point of the spherical surface is in an equal distance from the central point of the sphere. Another characteristic feature is that the sphere have the largest specific surface. In the inorganic macro- and micro-cosmos, and in organic, living structures, the sphere ("coccoid form") is very common.

As some selected example the following can be pointed out: PFLUG (1965a,b) in his first publications on the Precambrian biotas distinguished globular and filamentous structures. The extinctions on the K/T boundary are explained by KREMP (1990–91) by the expansion of the Earth. To this the "Pangean-polygon" of CAREY (1976) was an important hypothesis. The more or less isodiametric "Pangean-polygon" surface is composed of regular pentagons. Each pentagon increased by the same proportion. To this our, three dimensional modelling of the quasi-crystalloid skeleton was based on a pentagon dodecahedrane (KEDVES, 1990, 1991). The fullerenes which may serve as models for some biopolymer structures (cf. HARGITTAI, 1990) are quasi-equivalent systems (KEDVES and ROJIK, 1994). The quasi-crystals (SHECHTMAN, BLECH, GRATIAS and CAHN, 1984) may be interpreted with the PENROSE tiling (cf. PENROSE, 1979, NELSON, 1986). The quasi-crystalloid biopolymer structure was established in the plant cell wall (e. g.: KEDVES, 1990). The system is composed of a metastable skeleton, and a stabilizing system (KEDVES and TÓTH, 1994).

The aim of this paper is the modelling of the sphere with quasi-periodic elements, namely regular pentagons, and investigate the points of symmetry and the different kinds of holes (frustrations, sensu NELSON, 1986) of this system.

Methods

The computer modelling was made as follows:

1. Spherical calotte with the points of symmetry and the network of the regular pentagons (Text-fig. 6.1.).
2. The points of symmetry of the pentagons, and the central pentagon surrounding in two circles of pentagons (Text-fig. 6.2.).
3. The different kinds of holes and the central pentagon (Text-fig. 6.3.).

The interpretation of the computer data of the two dimensional schemes started from the central pentagonal plane of the calotte. In this way the analysis of the modelled characters may be serve in the reconstruction of the two dimensional schemes in the space.

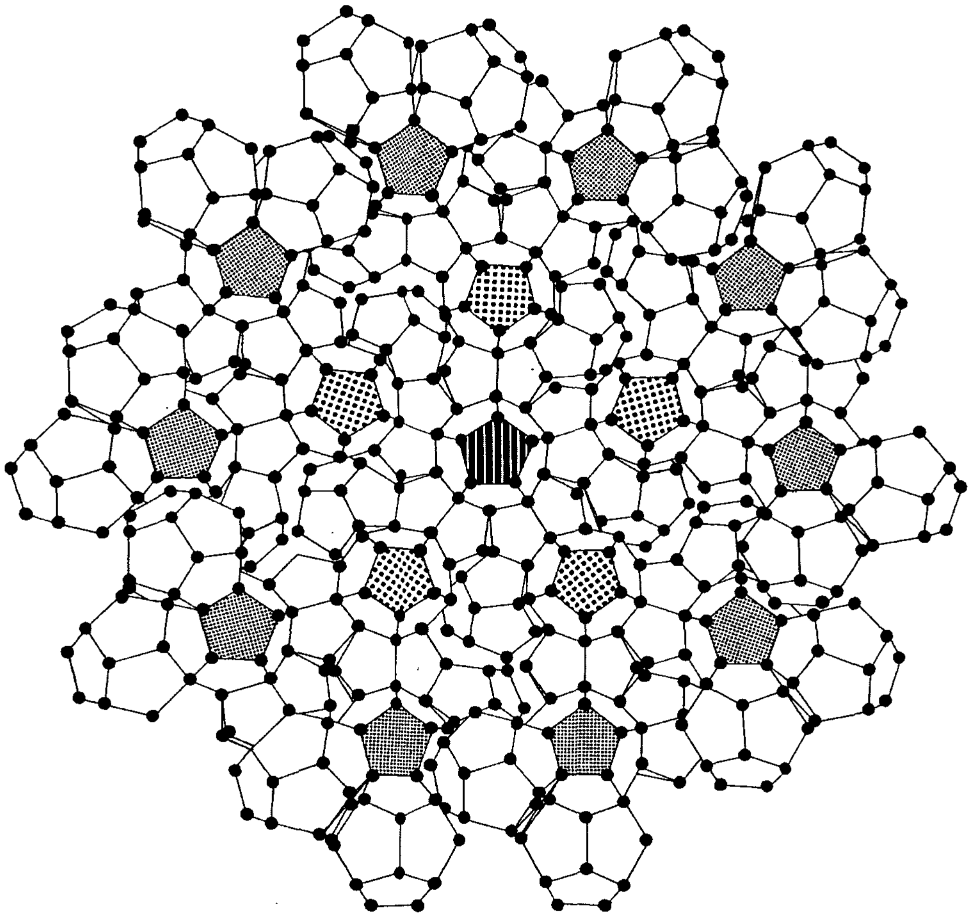
Results

1. PLANES, NETWORK AND POINTS OF SYMMETRY OF THE SPHERICAL CALOTTE (Text-fig. 6.1.)

1.1. The regular pentagonal planes

The central regular pentagon (streaked) is surrounded in two circles by further regular pentagonal planes. The first circle is composed of five pentagons (dotted with larger points) which are connected by its network to the edges of the central plane. The central pentagon which is effectively one side of the pentagon dodecahedrane, is surrounded by further pentagon dodecahedrane units. But in this case the five surrounding pentagonal planes are elements of a so-called "frustrated PENROSE-unit" in consequence of the forced quasi-equivalent arrangement of the quasi-periodic building elements. In the second circle of the regular pentagonal planes there are ten pentagons (dotted by tiny points). Each two of them is connected by one of their edges to the pentagons of the first circle. The pentagonal planes of the second circle elements of more frustrated Penrose units.

1.2. The network is composed of the sides of the regular pentagonal planes of the dodecahedranes which compose incontinuously the spherical calotte. This network well illustrates the peculiarity of this kind of spherical calotte. Namely the central pentagon is surrounded by ten edges, essentially this unit represents the central pentagon dodecahedrane. These points of symmetry are the bases of the ten pentagonal planes surrounding the central dodecahedrane. Each two surrounding pentagonal plane represents one unit, between them there are frustrations (sensu NELSON, 1986). The surrounding five pentagon represents also a dodecahedrane with minor positional differences to the central one. In contrast to these the pentagons of the second circle are peculiar, each second dodecahedrane is covered by another two



Text-fig. 6.1.

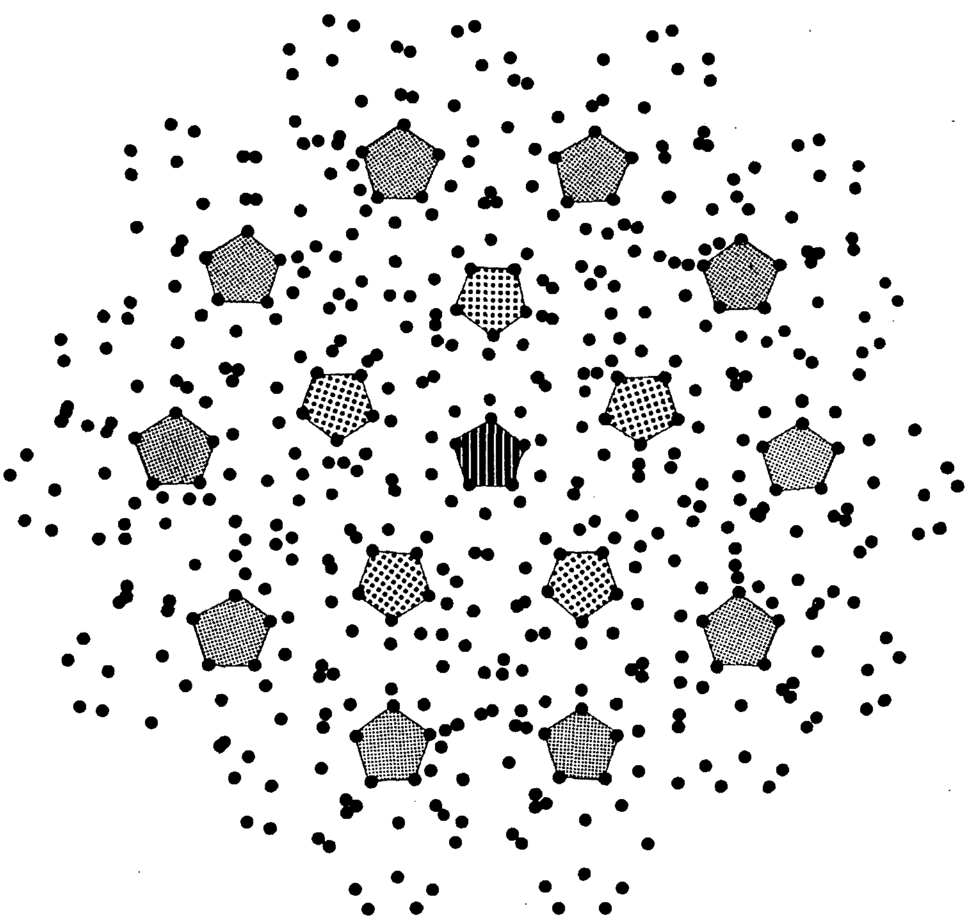
Scheme of the computer modelled spherical calotte composed of regular pentagonal planes. Illustrated are: 1. The central pentagonal plane (streaked) surrounded in two circles by further pentagonal planes (dotted). 2. The points of symmetry of the edges of the dodecahedrane. 3. The network of the superficial elements.

nearby pentagon dodecahedranes. In this way the points of symmetry surrounding the pentagonal planes of the second circle are the edges of two or three dodecahedranes. This phenomenon may be illustrated well by the symmetry of this points surrounding the regular pentagonal plane.

1.3. The points of symmetry are the edges of the pentagonal units. The points of symmetry together with the network lines well illustrate the position of the pentagonal planes which form the dodecahedrane elements. The disposition and/or the accumulation of the points of symmetry illustrate the position including the holes of the pentagon dodecahedrane elements.

2. PLANES AND POINTS OF SYMMETRY OF THE SPHERICAL CALOTTE (Text-fig. 6.2.)

The points of symmetry are the edges of the pentagon dodecahedrane units. The pentagonal planes are also illustrated as previously for orientation and for comparison to the previous figure (Text-fig. 6.1.). The network was omitted. The arrangement of the ten points of symmetry surrounding the pentagonal planes well represents the orientation of the dodecahedranes. Well shown is the regular position of the central pentagon. The ten points are on a regular circle. On the further circle of points there are also ten points, but paired. The twin points of the second circle are in the face of one point of the first circle. These three points represent



Text-fig. 6.2.

The points of symmetry of the edges of the dodecahedranes of the computer model of the spherical calotte and the pentagonal planes, illustrated in Text-fig. 6.1.

one kind of frustration between the dodecahedrane units. The further five single points of symmetry, near the second circle are opposite to the other five points of the first circle. These latter mentioned points are in the line of the edges of the two pentagonal planes respectively the central pentagon and one of the pentagons of the first circle. As regards the pentagonal planes of the first circle of pentagons, it is not so easy to establish the ten surrounding points of symmetry similarly to the central pentagon. This is in consequence of the space arrangement of the dodecahedrane units. These are in different kinds of arrangement. The peripherial units of the calotte are well represented by the points of symmetry of the edges of the pentagon dodecahedranes.

3. THE DIFFERENT KINDS OF HOLES AMONG THE BUILDING ELEMENTS OF THE SPHERICAL CALOTTE (Text-fig. 6.3.)

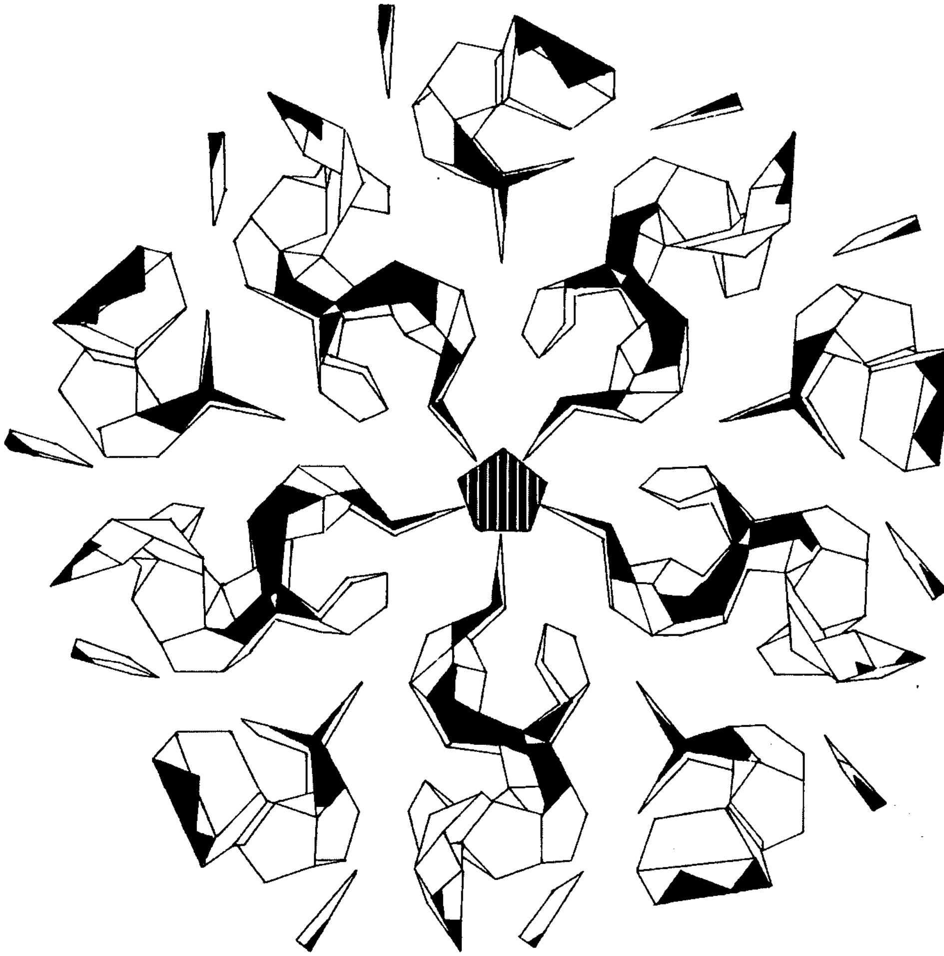
The holes among the building pentagon dodecahedrane units are superficial and internal. The superficial splits are illustrated in our figures by black fields, the internal ones by white fields. To a better understanding the orientation of the system of holes, the basic, central pentagon was also represented in this figure (Text-fig. 6.3.).

The superficial frustrations are very characteristic. The holes surrounding the central pentagon represent the frustrations of the PENROSE-unit of the quasi-crystalloid skeleton. The further ones are larger, and their form is altered in consequence of the arrangement in the space of the spherical calotte.

As regards the internal holes (frustrations sensu NELSON, 1986), a similar phenomenon can be observed near the central unit. The internal holes of the surrounding elements may be grouped into two types. Pentagons of oblique position can be recognized around the first circle of pentagons. Near the border of the spherical calotte several internal holes were demonstrated by the computer modelling with several pentagonal planes. Some of them are more or less similar in size and in position to the central pentagon. These holes are connected to the middle of the sides of the central pentagon. This represents the first system of holes.

The second system of the holes is not connected to the central pentagon, its pointed apices are oriented in the direction of the edges of the central pentagon. Five of such system of holes indicate further five pentagonal planes of the surface. Its arrangement is corresponding to the orientation of the spherical calotte.

Finally, there are further ten surrounding holes (superficial and internal together) in two kinds of orientation. Five are in opposition to one of the ending holes of the “second system of holes”. The other five are oriented more or less in the middle of the two systems of holes.



Text-fig. 6.3.

Computer modelled scheme of the superficial frustrations and the inner holes of the dodecahedrane elements of the spherical calotte. The superficial holes (frustrations sensu NELSON 1986) are indicated with black, the inner ones by white fields.

Discussion and Conclusions

1. As it was emphasized previously, this kind of structure modelled in this contribution was not observed directly on biological objects. On the other hand the globular form is extremely common and early at the biological structures.

2. The contradiction between the quasi-periodic and quasi-equivalent symmetries nearly the quasi-crystalloid and the buckminsterfullerene-like symmetries are well known. At our present modelling, the hexagons of the buckyballs were replaced by pentagons. In this way the surface of the spherical calotte and/or the surface of the total sphere is not complete it is full of holes.

3. Taking into consideration the presence of the quasi-periodic and the quasi-equivalent symmetries in living organisms, such kind of biopolymer structure of the biological objects may be presumed. The holes are supposedly filled by another kind of biopolymer structures.

Acknowledgements

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